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D. B. Harris, J. J. Zucca, D. B. McCallen, M. E.
Pasyanos, M. P. Flanagan, S. C. Myers, W. R. Walter,
A. J. Rodgers, P. E. Harben

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Considerations on the Use of 3-D Geophysical Models to Predict Test Ban Monitoring Observables

David Harris, Jay Zucca, David McCallen, Michael Pasyanos, Megan Flanagan, Stephen Myers, William Walter,
Arthur Rodgers, Phil Harben

Lawrence Livermore National Laboratory

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ABSTRACT

The use of 3-D geophysical models to predict nuclear test ban monitoring observables (phase travel times, amplitudes, dispersion, etc.) is widely anticipated to provide improvements in the basic seismic monitoring functions of detection, association, location, discrimination and yield estimation. A number of questions arise when contemplating a transition from 1-D, 2-D and 2.5-D models to constructing and using 3-D models, among them:

- 1.) Can a 3-D geophysical model or a collection of 3-D models provide measurably improved predictions of seismic monitoring observables over existing 1-D models, or 2-D and 2½-D models currently under development?
- 2.) Is a single model that can predict all observables achievable, or must separate models be devised for each observable? How should joint inversion of disparate observable data be performed, if required?
- 3.) What are the options for model representation? Are multi-resolution models essential? How does representation affect the accuracy and speed of observable predictions?
- 4.) How should model uncertainty be estimated, represented and how should it be used? Are stochastic models desirable?
- 5.) What data types should be used to construct the models? What quality control regime should be established?
- 6.) How will 3-D models be used in operations? Will significant improvements in the basic monitoring functions result from the use of 3-D models? Will the calculation of observables through 3-D models be fast enough for real-time use or must a strategy of pre-computation be employed?
- 7.) What are the theoretical limits to 3-D model development (resolution, uncertainty) and performance in predicting monitoring observables? How closely can those limits be approached with projected data availability, station distribution and inverse methods?
- 8.) What priorities should be placed on the acquisition of event ground truth information, deployment of new stations, development of new inverse techniques, exploitation of large-scale computing and other activities in the pursuit of 3-D model development and use?

In this paper, we examine what technical issues must be addressed to answer these questions. Although convened for a somewhat broader purpose, the June 2007 Workshop on Multi-resolution 3D Earth Models held in Berkeley, CA also touched on this topic. Results from the workshop are summarized in this paper.

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OBJECTIVES

The objective of this paper is to lay out technical considerations in the development and use of three-dimensional (3D) geophysical models for predicting the seismic observables used to monitor compliance with nuclear test ban treaties. These considerations could inform the structure of a program designed to develop a 3D model or models intended for operational use.

RESEARCH ACCOMPLISHED

Monitoring observables

For purposes of this discussion, the basic seismic monitoring functions consist of phase detection, phase association, event location, discrimination and characterization (i.e. magnitude and yield estimation). The potential seismic observables useful for these basic functions range from parametric data such as phase amplitudes, arrival times and surface wave dispersion characteristics (e.g. group delay) to derived waveform characteristics such as the coda envelope, to, in some cases, the full seismic waveform. Treaty monitoring is carried out at local ($< \sim 200$ km), regional ($< \sim 2000$ km) and teleseismic ($> \sim 2000$ km) distances. The principal phases are P, S and surface waves (Rg) at local distances, and Pn, Pg, Sn, Lg and the surface waves (Rayleigh, Love) at regional distances (Figure 1). A very large number of phases are available for monitoring purposes at teleseismic ranges, though the principal phases that are intensively calibrated are the first arriving P and S, and surface waves.

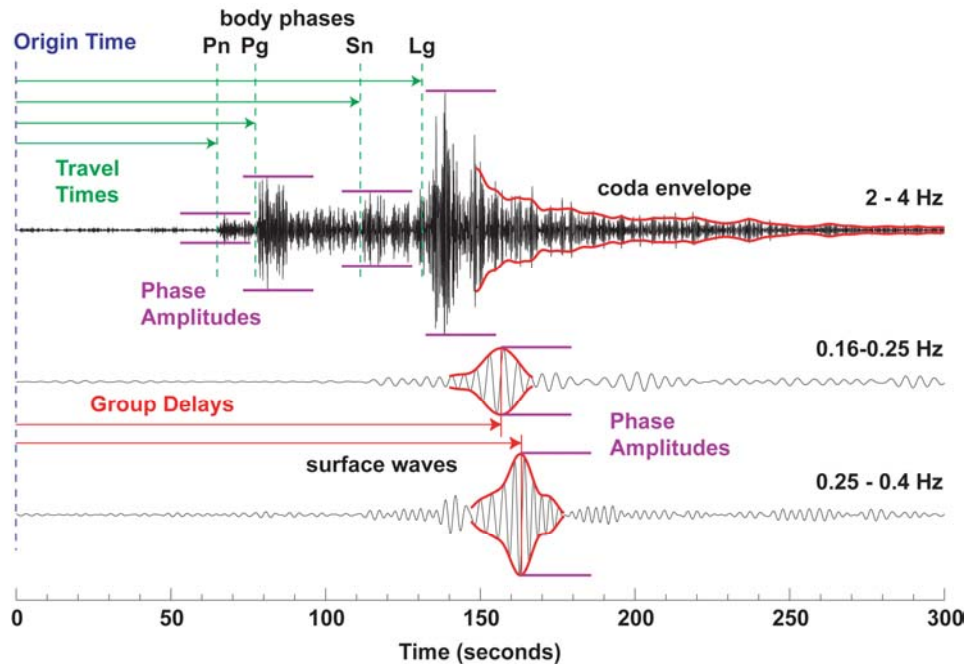


Figure 1. Principal parametric observables at regional distances consist of arrival times and amplitudes of the 4 major phases (top trace) Pn, Pg, Sn and Lg, and dispersion characteristics of long and short period surface waves (bottom traces).

One of the most important factors affecting the development and use of 3D models (principally through the required resolution of the models) is the frequency band in which monitoring observables are measured. The nuclear test monitoring band extends from 20 seconds (for Ms, magnitude measurements from surface wave amplitudes) to 10 Hz or even higher (for body wave amplitude measurements used in discrimination and arrival time picks used in location). Sufficient data are not available to constrain 3D models sufficiently to make accurate predictions of waveforms at the high-frequency end of this spectrum. However, stochastic models may be developable that may predict bulk characteristics of seismic waves, such as amplitude and coda shape.

Modeling objectives: accuracy, operational considerations

Seismic events are detected and interpreted by a process of matching observed signal characteristics with characteristics predicted by a model from trial values of the principal event parameters: location, origin time, magnitude, mechanism and source time history. Often the process is iterative, as indicated in Figure 2. The process drives the residuals (differences) between predicted and measured values as close to zero as possible. Usually station corrections for each predicted observable are developed from observations of ground truth events. Station corrections can be appreciable where models (whose geophysical parameters vary relatively smoothly compared to the earth) fail to predict observables closely enough. Station corrections typically take the form of maps of residual bias (variation from zero) as a function of latitude, longitude (and sometimes depth) of the sources observed by the station.

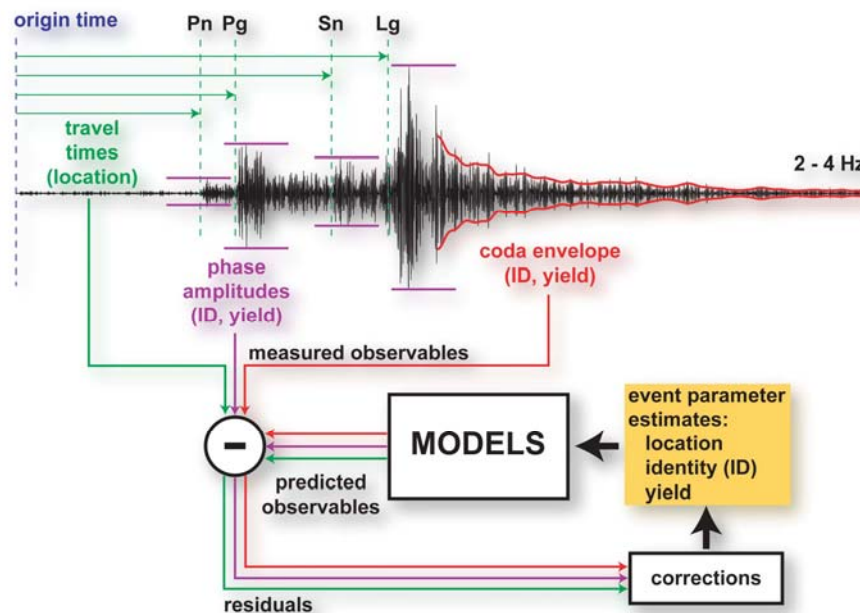


Figure 2. Models form the core of an iterative process of predicting observed signal characteristics (parameters, envelopes, waveforms) in order to detect, locate, identify and characterize seismic events.

The physical parameters comprising the models include compressional (P) and shear (S) velocities, intrinsic attenuation for both P and S and medium density. In a 3D model, these parameters would be mapped as a function of latitude, longitude and depth from the surface. Additional, higher-order physical parameters such as anisotropy may need to be considered as well.

It is desirable to concentrate as much as possible of the predictive capability of this system in the model, since the model will provide predictions for stations that do not have empirical corrections either because the stations are newly deployed or because they observe relatively aseismic regions. Clearly, one of the principal objectives in building a model is to make predictions derived from it as accurate as possible.

However, accuracy is not the only objective. The models of interest to the monitoring community are intended to be embedded in pipelines detecting and interpreting events from real-time data streams. Consequently, calculations of observables from the models must be fast enough to keep pace with a real-time system. Often, as is the case with location, predictions of observables must be made repeatedly when interpreting a single event as the estimation algorithm iterates to a solution from a starting estimate. Hundreds or thousands of evaluations of observed parameters may be required to interpret a single event. This requirement implies, for example, that travel-time estimates be calculated in just milliseconds.

Geographical coverage is another issue; global capability is required, but especially good predictions are desirable in Eurasia and Africa.

In addition, the predictions made by models must be seamless. Heretofore, highly accurate local and regional observable (e.g. travel-time) models have been spliced together to form a single model spanning a large (global or continental) region. This practice sometimes has led to boundaries between regions with offsets in the predicted observables. These offsets have been somewhat artificially or arbitrarily smoothed together to avoid presenting discontinuities to estimation algorithms. A desire to avoid such discontinuities is driving the monitoring community toward development of increasingly geographically comprehensive models, ideally embedding high-resolution regional geophysical models seamlessly in global models. There is a spreading consensus that any blending or splicing that needs to be done, should occur in the geophysical models and not in the derived predictions of observables. Because of the heterogeneity of regions, comprehensive geophysical models are necessarily going to be at least 2D and more generally 3D.

There is a question as to whether 3D models will provide sufficiently improved accuracy to justify the added cost of developing them and the pipeline support to use them. It is clear that a patchwork quilt of 1D models is not sufficiently accurate, particularly around boundaries among regions described by distinct 1D models where discontinuities are an issue, and by defaulting to iasp91 in regions where no data are available. They also are complex to implement and maintain. Currently the NNSA labs and AFTAC are engaged in building 2.5D approximations to 3D models for predicting regional phase travel times. These are planned to be tomographic models, which should be seamless and provide greater predictive accuracy than 1D models everywhere, including in aseismic regions.

One model or many?

Previous seismological practice in model building was to construct separate models for each observable to be predicted, and generally to use data of the intended observable to invert for the model. Hence, body wave travel-time observations were used to construct predominantly P velocity models and surface wave dispersion data to construct shear wave models. These models often had their best resolutions at different depths due to the fact that body phases sample the earth (travel) deeper than surface waves. Measurements made from disparate wave types represent different averages of often distinct geophysical parameters.

Current practice, especially in global tomography, is to perform joint inversions of several or even many data types to estimate one or often several geophysical parameters. The use of multiple data types improves coverage by providing constraints at different depths and observations over a larger number of (great circle) paths.

While the desirability of inverting many data types simultaneously to produce models is generally accepted, a question remains about whether to strive for a single model to predict all observables or individual models to predict each observable separately. A single model is desirable for operational and maintenance simplicity, but it may be that dedicated models will have greater prediction accuracy, especially if they employ specialized representations for the observable in question (such as dispersion maps for surface wave group delay predictions instead of P and S velocity models).

Model representation, uncertainty

There are a number of separate issues to be resolved that fall under the general heading of model representation. While not necessarily unique to 3D models, these issues are exacerbated by “the curse of dimensionality,” the rapid increase in complexity, and storage and computational requirements in the transition to 3D representations.

The first issue is the mathematical form of representation for any particular geophysical quantity. Options include sampling the quantity on a regular geographic grid of points or cells, sampling on a tessellated mesh, and representation in terms of the coefficients in a basis function expansion. Often models are described most simply as a stack of layers in depth in latitude-longitude cells; the parameters are layer thicknesses, P and S velocities, intrinsic Q for P and S waves and medium density.

One consideration for the choice of representation is the fidelity of the model to the earth it represents. Model fidelity is influenced by the resolution of the representation and the accuracy of suitable interpolation schemes.

Generally, the greater the resolution, the more accurate the representation (especially of boundaries) and the larger the space required to store the model. The accuracy of the model, however, is most fundamentally limited by the coverage of the data used to construct it.

A solution, almost sure to be employed in development of large 3D models, is the use of multiple resolutions. The model may be very dense in the shallow regions of the crust and lithosphere, where heterogeneity is greatest and more accurate predictions of rapidly-varying observables is desired. The model may be sparse in the deeper, more homogeneous mantle and core. In the nuclear test ban application, some geographic regions will be more accurately and finely represented than others of lesser importance.

A second consideration is the accuracy of the waveform or parameter observable generated by forward calculation through the model. Computed observable accuracies may require resolutions that exceed those required for model fidelity. Numerical requirements may dictate sampling densities as high as ten times per wavelength, often much more finely sampled than justified by available constraints on the model implied by available data. The choice of model representation often significantly influences numerical accuracy, as can happen with the superior definition of reflecting boundaries finite or spectral element methods.

A third and related consideration is the speed with which observables can be calculated through the model. Many algorithms required extraction of earth model quantities along great circle paths or along more arbitrary paths (as with full ray tracing). Such algorithms place a premium on fast interpolation methods, since they require geophysical parameter values at points generally not coincident with mesh or grid sample locations. Tessellation meshes have to be “walked” to find the specific tetrahedra where model values are required. Efficiency of model interrogation and interpolation, accuracy and model storage requirements may trade against each other.

The second major issue is the estimation and representation of model uncertainty. In current practice, the majority of models, even the vast majority, are deterministic. Where uncertainties in model parameters are estimated and reported at all, usually Gaussian statistics are assumed and model parameters are described as the mean of the distribution. The variance may be estimated from *a priori* considerations of normal geophysical variation, or more robustly through a statistical procedure such as the jackknife or bootstrap during inversion. Although variations among different model parameters are almost certainly correlated, covariance estimates are not commonly reported.

Stochastic geophysical models are an attractive though computationally- and storage-intensive alternative (particularly in 3D) to deterministic models. Stochastic models represent uncertainty with a collection of thousands of realizations that provide a posterior distribution on sample models that are consistent with available data (see e.g. Figure 3). The density of sample models in the model parameter space constitutes an approximate probability distribution on the model that can be used to extract moments (mean model, variance) that characterize uncertainty. This representation easily embraces non-Gaussian, and even multi-modal, statistics. Relatively efficient grid-search methods exist to produce the collection of realizations that constitute a 3-D stochastic model by fitting simultaneously a variety of observation data. However, large-scale computing is required to check the thousands of representative sample 3-D models against available data by predicting a variety of observables (surface wave dispersion, body-wave travel times, receiver functions, etc.). Stochastic models of this sort readily allow the estimation of uncertainty in predicted observables, since multiple estimates of the observables can be obtained by forward calculation through the suite of sample realizations. The result is a distribution on the observables, as shown in Figure 3.

A priori model development

Geophysical models can be developed in several ways, including the compilation of existing information from diverse sources such as maps, general physical constraints on earth structure and specific geologic descriptions from prior studies into *a priori* geophysical models. Figure 1 below, shows various aspects of a unified 3D geophysical model of Eurasia and North Africa developed by the NNSA labs. LLNL constructed the western half of the model, which is designated the WENA (Western Eurasia, North Africa) model. The WENA model is compiled from a large number of literature sources. A priori models are useful in themselves, but also may serve as the starting point for the other major class of models, tomographic models, often as Bayesian priors. Tomographic models are obtained by inverting mathematically observations of phase travel times, amplitudes, dispersion and other characteristics over many crossing paths to constrain the 3D velocity structure and other model parameters.

Model validation

Model validation is an essential component of all model development and acceptance as it tests the predictive capabilities of a model. The fundamental steps of validation are the same as in model estimation from data: (1) collection of ground truth information on events for which seismic observables can be measured, (2) development of procedures to predict those observables through the model, (3) collection of waveform or other data from which to measure observables, (4) making the measurements and (5) comparing the measurements with the model predictions. The additional step in model construction not performed in validation is adjusting the model parameters in an iterative process to better match the measurements.

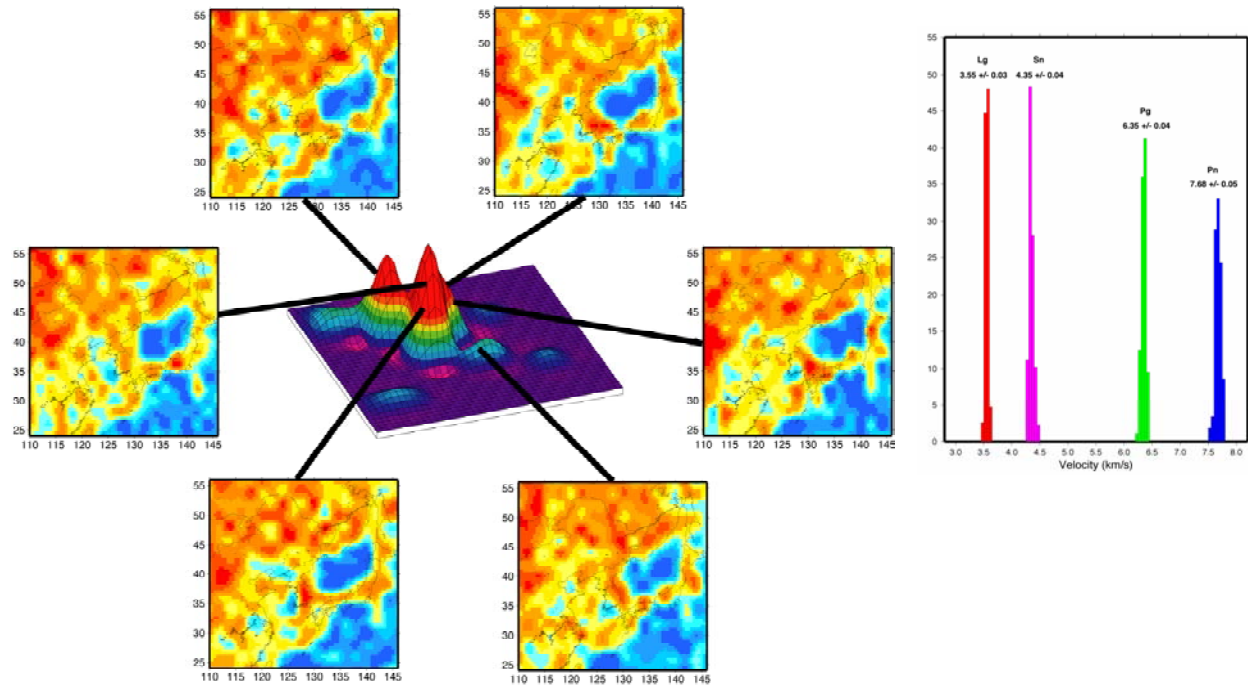


Figure 3 Six realizations from a 3D stochastic geophysical model surrounding the Korean peninsula demonstrate the concept that the uncertainty for the model is captured by a probability distribution represented by the density of realizations in model space. At upper right, distributions for predicted travel-time observables along a specific path show the ability of this type of model to predict uncertainties in monitoring observables.

An example of travel-time model validation is shown in Figure 5 for the WENA model. In this case, the model is used to predict first P arrival times. Since this is a 3-D model, the travel times are predicted with a 3-D finite-difference code solving the eikonal equations. This assessment shows that even an *a priori* 3-D geophysical model improves travel time predictions compared to a standard (iasp91) 1-D earth model.

Validation of tomographic (data-driven) models presents a dilemma: how much of the available ground truth information and measurements should be used to develop the model and how much should be held out to perform validation. To prevent circularity problems, the same data cannot be used for both functions. Cross validation and similar statistical sampling techniques can obviate this problem at added computational cost. The problem becomes particularly acute in the development of 3D models, because the added dimension of such models mean that many more model parameters must be estimated, and more and more data are required to constrain the estimates.

Data types required for the inverse problem

In this paper, we use the term “inverse problem” to mean the problem of estimating geophysical model parameters from seismic and other observables. By contrast, the forward problem is that of predicting the observables from an extant model. The data types required or available to solve the inverse problem are many and varied. They include

measurements of the observable types that the models are intended to predict: P and S absolute and differential travel times, P and S wave amplitudes, surface wave dispersion. They also include other types of data that provide additional, often complementary constraints: receiver functions, structural constraints from refraction and reflection seismology, gravity anomaly data from satellite orbital perturbations, heat flow, normal mode peak splitting, constraints from geologic or tectonic interpretations, to name some of the more important types.

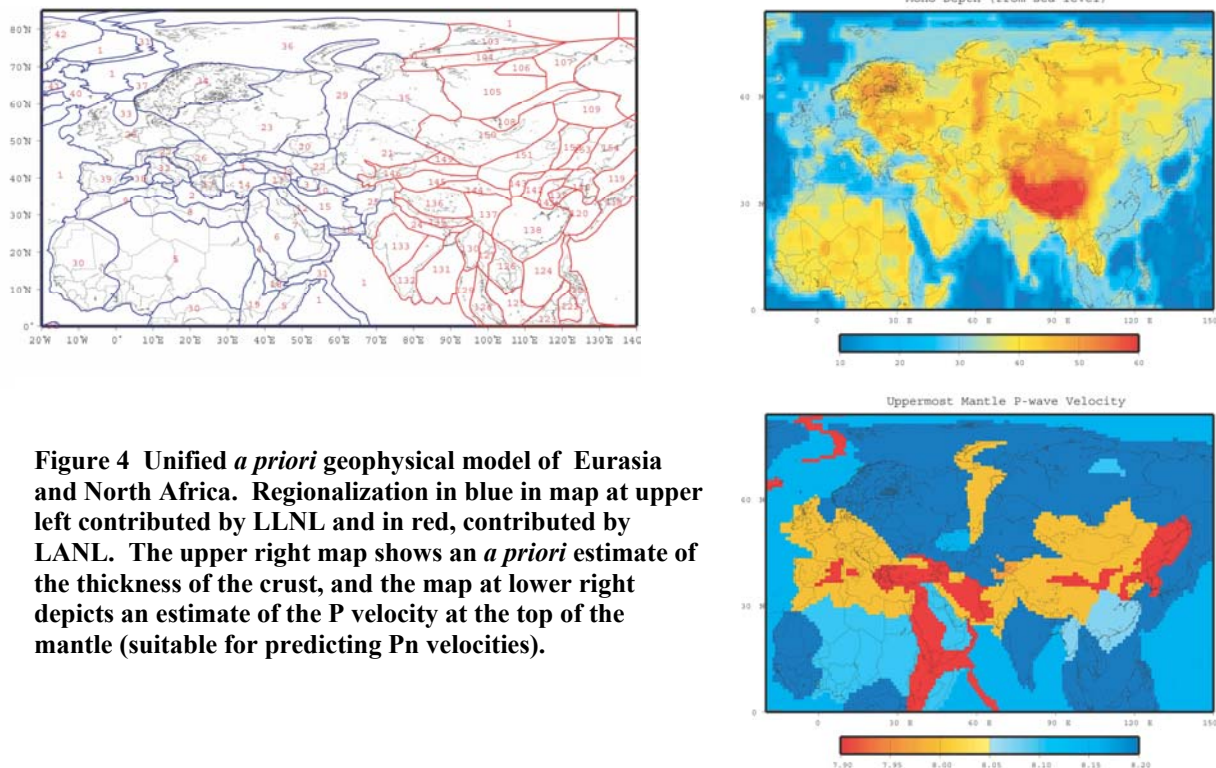


Figure 4 Unified *a priori* geophysical model of Eurasia and North Africa. Regionalization in blue in map at upper left contributed by LLNL and in red, contributed by LANL. The upper right map shows an *a priori* estimate of the thickness of the crust, and the map at lower right depicts an estimate of the P velocity at the top of the mantle (suitable for predicting Pn velocities).

As mentioned earlier, different data types result from waves or fields that sample different portions of the earth and do so with different weighting or averaging over the regions to be model (expressed as different resolution kernels in inverse methods). The issue for developing large-scale 3D models is again the curse of dimensionality – 3D models have many more parameters to estimate than 2D or 1D models. The larger and more varied the volume of data brought to bear on the problem, the more certain will be the result and the better the resolution (within limits set by the distribution of stations and sources).

Path Coverage and Data Quality

Data coverage and quality issues are among the most important practical considerations when contemplating the construction of 3D models. For those data types that are seismic observables, the distribution of paths sampling the volume of the earth is not under our control. Events are not uniformly distributed, but highly concentrated along plate boundaries. Stations are not uniformly distributed either, because of the fact that land mass constitutes only 30% of the earth's surface, and many regions are inaccessible for political reasons.

The number of events available to provide data for model building is further constrained by quality requirements. Especially for constraining the velocities of models from seismic wave travel-time observations, the locations, depths and origin times of events have to be known accurately. This has led to requirements on ground truth information, generally designated as GTx, where “x” specifies the uncertainty in the location of the event, e.g. 1 km, 5 km, 25 km. A significant issue for the development of 3D models is that the number of events with the most desirable ground truth levels (GT5 or better) is in the low thousands, whereas the total number of events reported in

major bulletins is in the many hundreds of thousands. The development of high quality ground truth information remains a priority for model development.

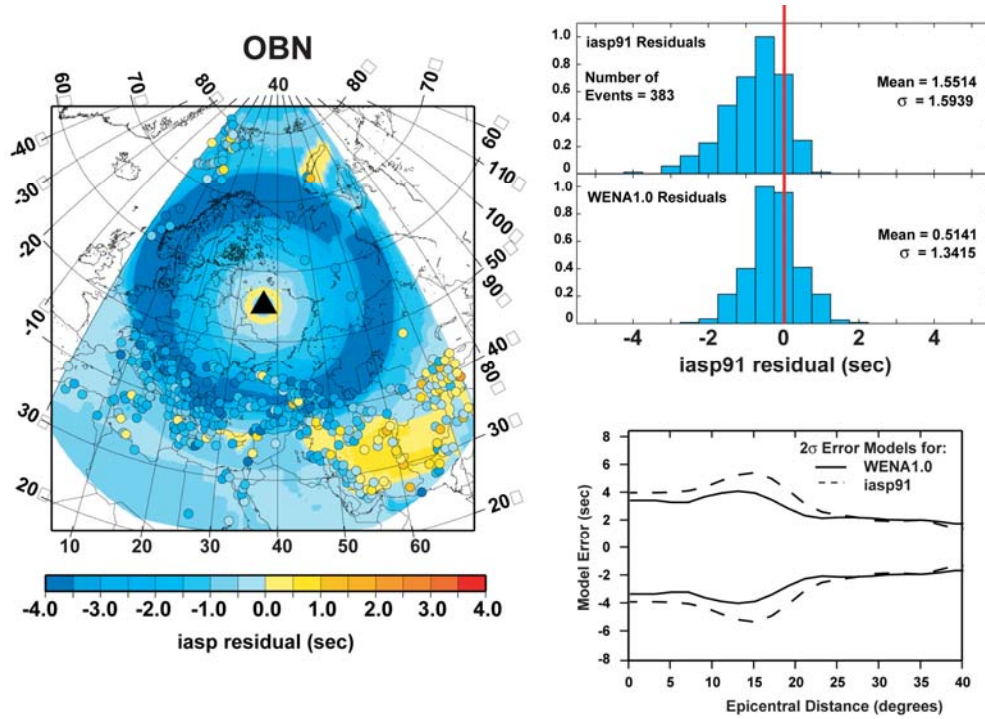


Figure 5 Observed travel-time residuals at station OBN (Obninsk, Russia) against predictions from the 1-D iasp91 model. At left, the measured (color coded) residuals against iasp91 predictions are plotted as points, superimposed on a surface representing the difference between the 3-D WENA model prediction and the iasp91 prediction. Note that the *a priori* WENA prediction correlates well with the measured residuals. Summary statistics at right show that the WENA residuals are closer to zero mean and have smaller variance than the iasp91 residuals.

The inverse problem: objective functions and inversion methods

From what we have discussed so far, we see that the 3D models of interest to the monitoring community ultimately are likely to be global, multi-resolution models with considerable detail at shallow depths in certain continental regions and less detail under the oceans and in the deeper mantle and core. Development of such models will make extensive use of *a priori* constraints to offset, to the degree possible, the relatively insufficient (though still very large) quantity of data available to estimate model parameters. To minimize pipeline complexity and maximize software maintainability, there will be pressure to consolidate predictive capability into as few separate models as possible, ideally into a single model. The model or models that emerge will be multifaceted, representing simultaneously many or all geophysical parameters of interest and predicting many or all monitoring observables. Correspondingly, many disparate data types will have to be inverted simultaneously to estimate the model parameters.

This inversion problem represents a significant challenge. A number of factors will have to be addressed simultaneously in deciding a suitable inversion technique: the mathematical objective functions used as figures of model merit (including the related statistical descriptions of prediction residuals), whether parametric or waveform data will be fit, the resolution of the model, the computational and storage requirements.

The statistics of the residuals (Figure 2) between model predictions and data will largely drive the objective functions. If Gaussian statistics are adequate, then least-squares objectives may be indicated. If correlated residuals are likely, then an objective function with suitable covariance structure will be required. If non-Gaussian or multimodal statistics are likely, then a grid-search approach might be required, such as a Markov-Chain Monte

Carlo (MCMC) method. A multiple objective approach (next section) might be superior when several disparate observables are predicted by the same model. *A priori* constraints on the models may suggest Bayesian objective functions.

The choice of inversion engine also may be driven by the desirability of performing constrained optimization. Physical constraints (realistic ranges of velocities and densities, or rheological conditions, for example) may require penalty function, barrier function, interior point or other constrained optimization techniques.

If stochastic models are desired, as may happen if a realistic exploration is required of model tradeoffs and parameter correlations, then a sophisticated grid search (MCMC, simulated annealing) will be necessary. These options almost surely will require large-scale computing to construct 3D models.

Development of even deterministic 3D models with global coverage will require large amounts of computer storage and speed. A typical model might be hundreds of megabytes or even larger. If fitting full waveforms, or some functionals of waveforms (e.g. envelopes) in the higher frequency bands of monitoring interests becomes important, then model prediction of observables (waveforms) will require computers with hundreds or thousands of processors. If stochastic sampling approaches are employed, then storage for thousands of models will be required. The inversion problem then would be in the terascale or petascale range.

June 2007 3D Model Workshop

On June 6 and 7, 2007, LLNL hosted a workshop on the future of 3D models in seismic monitoring and hazard applications. The objective of the workshop was to bring together government, industry and academic leaders in the development and use of geophysical models to predict seismic observables for monitoring and hazard applications to explore issues surrounding the transition to 3D models. Several trends favoring 3D models are converging: the continued proliferation of digital seismic stations globally and the general availability of data from these stations, the decreasing cost of computer storage and processing power, and the increasing sophistication of modeling techniques. Here is a list of presentations at the workshop and a few comments on each.

Comments on the use of 3-dimensional models for monitoring (D. Russell, AFTAC)

AFTAC has a different objective from than hazard: it wants to understand the source, not effects on structures. The monitoring community seeks a unified global model, possibly 3D, and one that can serve all communities. The jury is out yet on 3D models: can they really improve on 2.5D approximations currently under development?

Key observables for monitoring hazard: the prospect of using 3D models to improve prediction (A. Rodgers for D. McCallen, LLNL)

Historical simulations for hazard assessment focused on single problem components (source characteristics, propagation, soil-structure interaction, structural response) with simplifying idealizations. A 3D simulation of all components in a single end-to-end process would significantly improve predictions.

Building a better SF Bay Area model (T. Brocher, USGS)

The USGS has built an *a priori* 3D model for the San Francisco Bay Area incorporating velocity, density and intrinsic attenuation and is using it to predict strong ground motions from different fault rupture models. Velocity discontinuities are a crucial feature for accurate predictions. Extensive model validation is underway.

The evolution of global and regional models (M. Pasyanos, LLNL)

The seismic community has been very successful at producing models meeting individual disparate needs, but less successful at producing models meeting a variety of needs. The history of model development was summarized and the characteristics of a desirable monitoring model were described.

Representation of Global Earth Models: efficiency, interoperability and prediction accuracy (W. Menke, LDEO)

Interoperability among models (supporting the use of one researcher's model by other individuals) is a problem for the community. Model authors need to state what data are fit by their models and how well to support use by others.

Toward seismic tomography based upon adjoint methods (J. Tromp, Caltech)

Adjoint methods using full-waveform 3D synthetics offer the most realistic methods for estimating structure to date, as they properly account for finite-frequency effects. Increases in computing power are making adjoint tomography feasible, with global simulations in the 1-2 Hz range on the horizon with petascale computing.

Near-regional tomography in Northern California (C. Thurber, U. Wisconsin)

A consortium is developing a high-resolution tomographic model of California using observations from many hundreds of stations, forward travel-time predictions made with finite difference solutions to the eikonal equations and double-difference tomography. A spherical finite difference solver is in development. Next steps may include the use of global and regional data.

Recent advances in ambient noise tomography (M. Ritzwoller, U. Colorado)

Ambient noise tomography produces striking high-resolution 3D shear velocity models of the crust and upper mantle using long-term correlations of ambient noise among stations of a network. The method produces empirical Green's functions that may find application in an innovative type of event location.

Combining complementary data to constrain regional Earth models (C. Ammon, Penn State Univ.)

Simultaneous inversion of several types of data provides better constraints on structure. Example: joint inversion of gravity and surface wave dispersion. Gravity constraints preserve sharp horizontal boundaries typically lost in seismic tomography. Multiple objective optimization (MOOP) enables trades among simultaneous objectives.

Global tomography overview (P. Shearer, Scripps Inst. Of Oceanography)

The current emphasis in global model development is on fitting multiple types of data. Data coverage is paramount; theoretical and inversion considerations play a role but are less important. Current methods assume a simple crust, but the crust often is the largest source of variations in teleseismically observed travel times used for tomography.

The Future of High Performance Computing (D. Kusnezov, NNSA)

The DOE is pursuing weapon simulation with petascale computing to replace underground testing with a scientifically rigorous methodology to assess and maintain confidence in the nuclear stockpile. This effort is driving the development of supercomputing with applications that extend to scientific discovery in many other disciplines.

Three-dimensional simulation in seismic hazard assessment for engineering practice (N. Abrahamson, PG&E)

There is a major gap between simulation and engineering practice in structural design for seismic hazard. Huge variations in simulation results done by different research groups and the fact that practicing engineers cannot run the simulations themselves are barriers to acceptance. Acceptance of model simulations is 5-10 years out.

End-to-end earthquake modeling: From 3D ground motion to structural performance, including soil-structure interaction (J. Bielak, Carnegie Mellon Univ.)

The end-to-end strong-motion simulation problem (from source to structure) is difficult to analyze as a whole. A domain decomposition approach treating the problem in different scales is feasible and producing very interesting results showing that structure-structure interaction by coupling through the soil is a significant factor.

Non-linear source modeling and coupling to linear codes (T. Antoun, LLNL)

Non-linear modeling of strong-shock physics is producing ever more realistic simulations (matching available data) in the near-source region. Coupling to linear codes through a domain decomposition (boundary condition matching) approach will enable simulations of regional seismic observables of nuclear explosions.

Modeling regional broadband arrays (D. Helmberger, Caltech)

Better estimates of event mechanism and location are obtained with a hybrid technique of computed synthetic waveforms with unmodeled structural effects empirically calibrated against well-constrained training events. The amplitude and phase calibrations are made on portions of the waveform partitioned by (up/down) ray parameter.